MPI Version of the Serial Code with One Dimensional Decomposition

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Overview

We will choose one of the two dimensions and subdivide the domain to allow the distribution of the work across a group of distributed memory processors

We will focus on the principles and techniques used to do the MPI work in the model

STEP1: introduce the MPI environment

10 minutes

- cd /mpi_1d/step1
- compile and run the serial code
- edit the file step1.f : (only the main program)
  - include the mpi header file
  - declare integer variables size, rank, ierr
  - initialize MPI
  - determine process group size
  - determine the rank of calling process
  - terminate MPI environment

STEP1: introduce the MPI environment (continued)

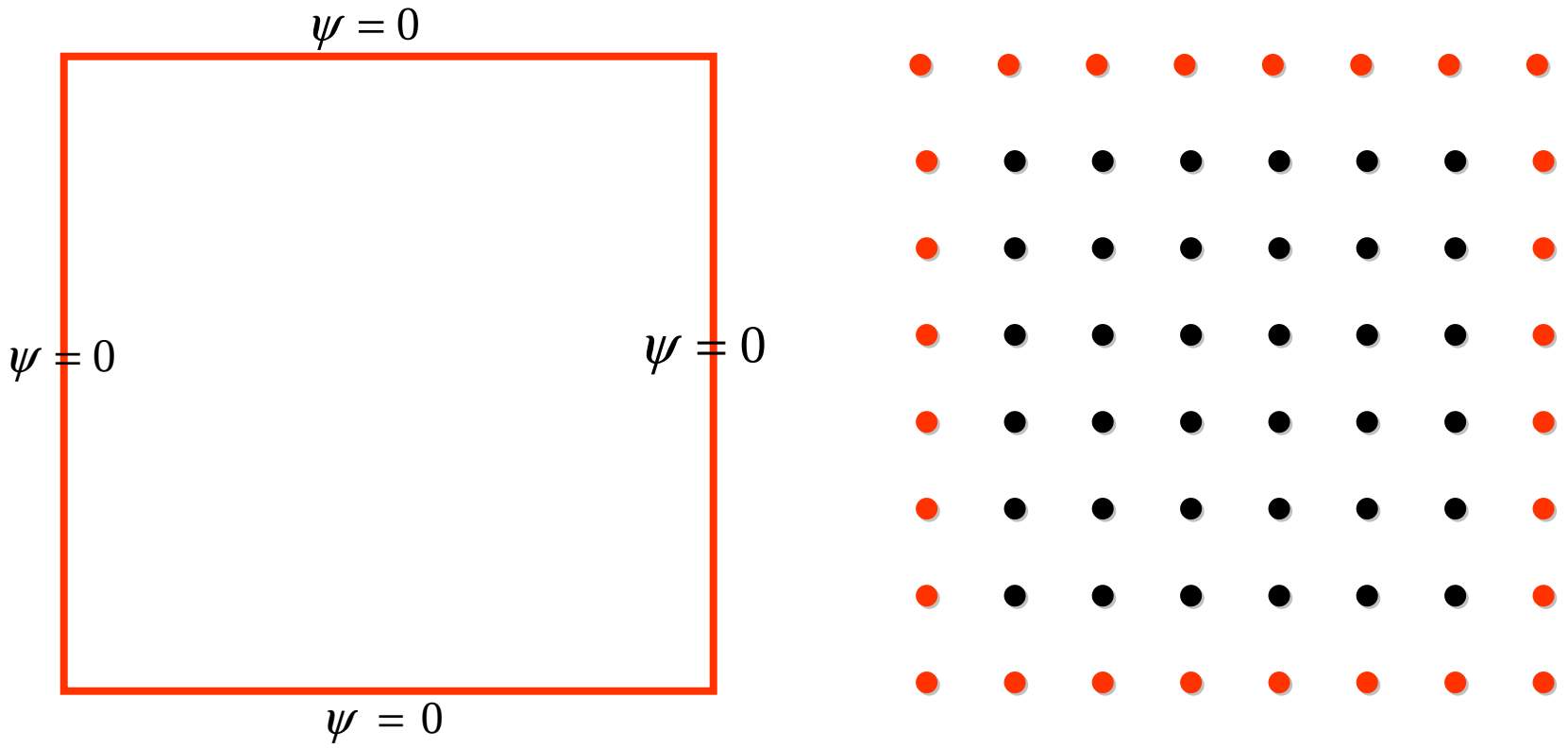
- compile step1.f :

  mpif77 step1.f -o step1.x

- run the executable on one processor

  mpirun -np 1 step1.x

Domain Discretization



Structure of the Serial Code

- namelist : Lx, Ly, α , β, γ
- grid : Δx, Δy
- forcing : $- \alpha \sin(\pi * (j-1) * \Delta y / Ly)$
- initial : $\psi(i, j) = 0.0$ for $i = 1, nx, j = 1, ny$
- bcs : $\psi(i,1) = \psi(i,ny) = \psi(1,j) = \psi(nx,j) = 0$

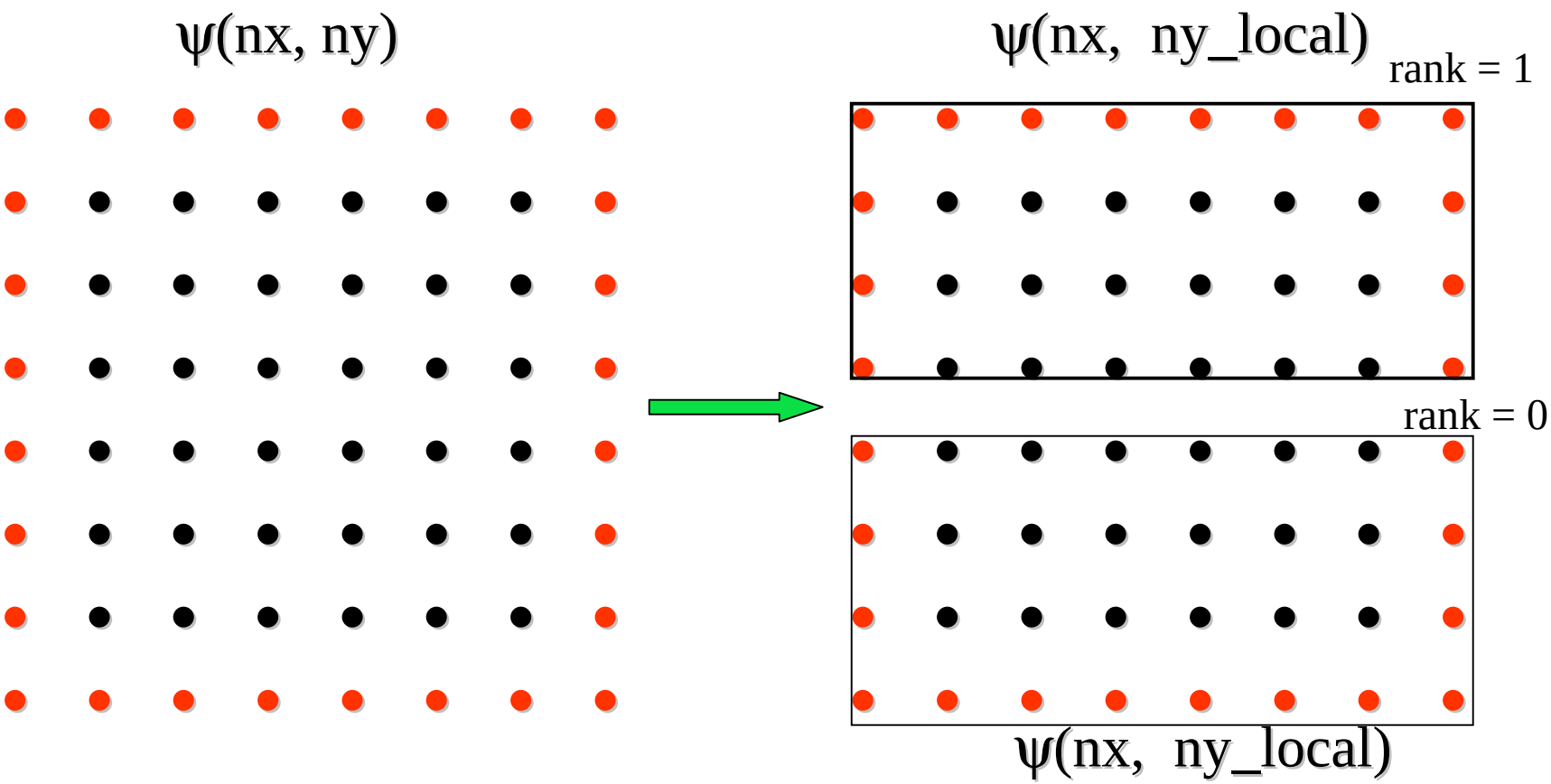
Structure of the Serial Code (continued)

begin iteration: it = 1, itcnt

- jacobi : $\psi\_new(i, j) = a1*\psi(i+1,j) + a2*\psi(i-1,j) + a3*\psi(i, j+1) + a4*\psi(i, j-1) - a5*f(i, j)$; i=2,nx-1,j=2,ny-1
- residual : $(\psi(i,j) - \psi\_new(i, j))**2$; i=2,nx-1,j=2,ny-1
- copy : $\psi(i,j) = \psi\_new(i, j)$
- end iteration

ID Decomposition

Physical domain is sliced into slabs so that computation in each slab will be handled by different processors.

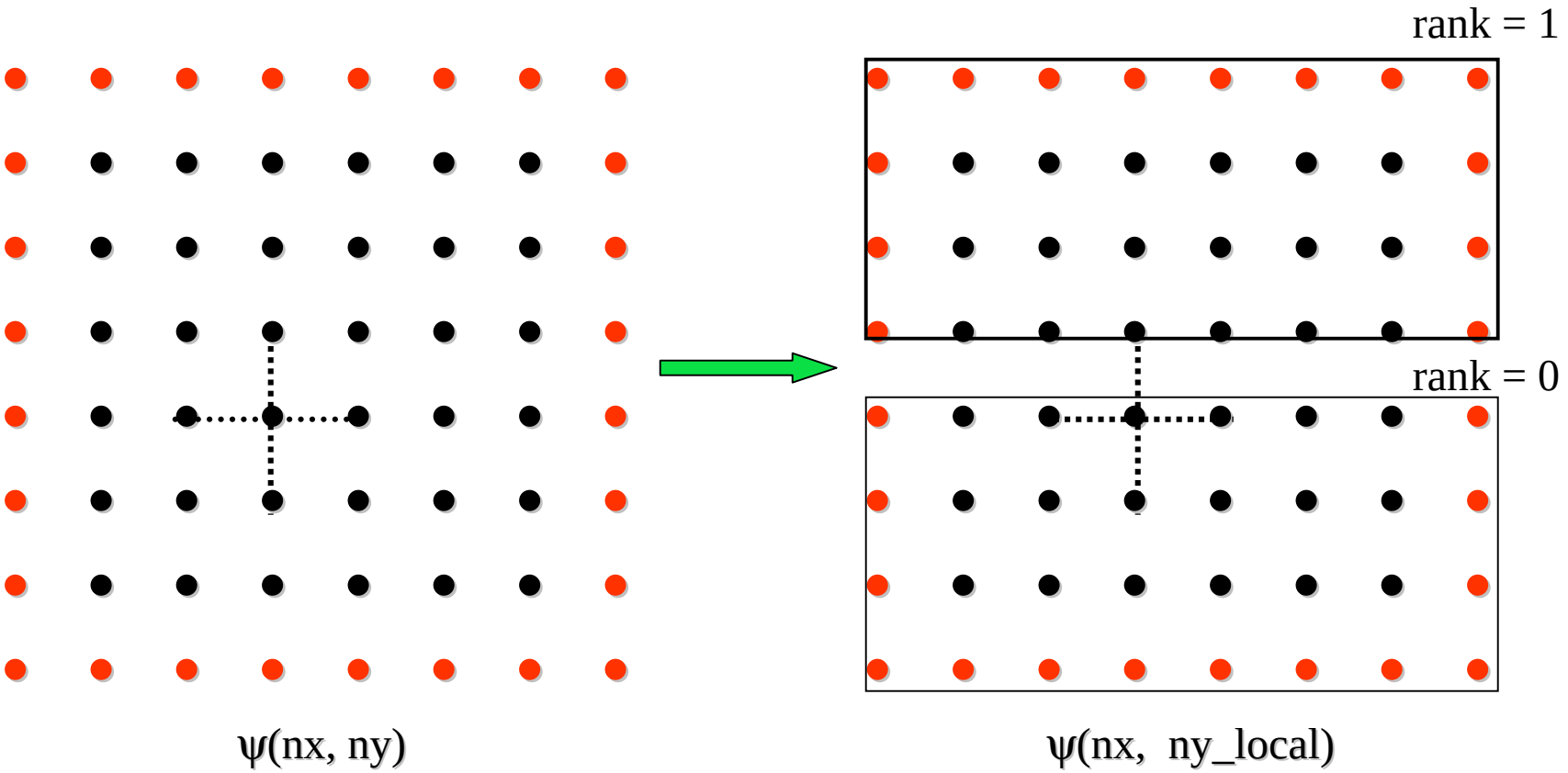


Jacobi Iteration on Decomposed Data

$$\psi\_new(i, j) = a1*\psi(i+1,j) + a2*\psi(i-1,j) + a3*\psi(i, j+1) + a4*\psi(i, j-1) - a5*f(i, j)$$

i=2,nx-1 ; j=2,ny-1

i=2,nx-1 ;j=2,ny_local-1



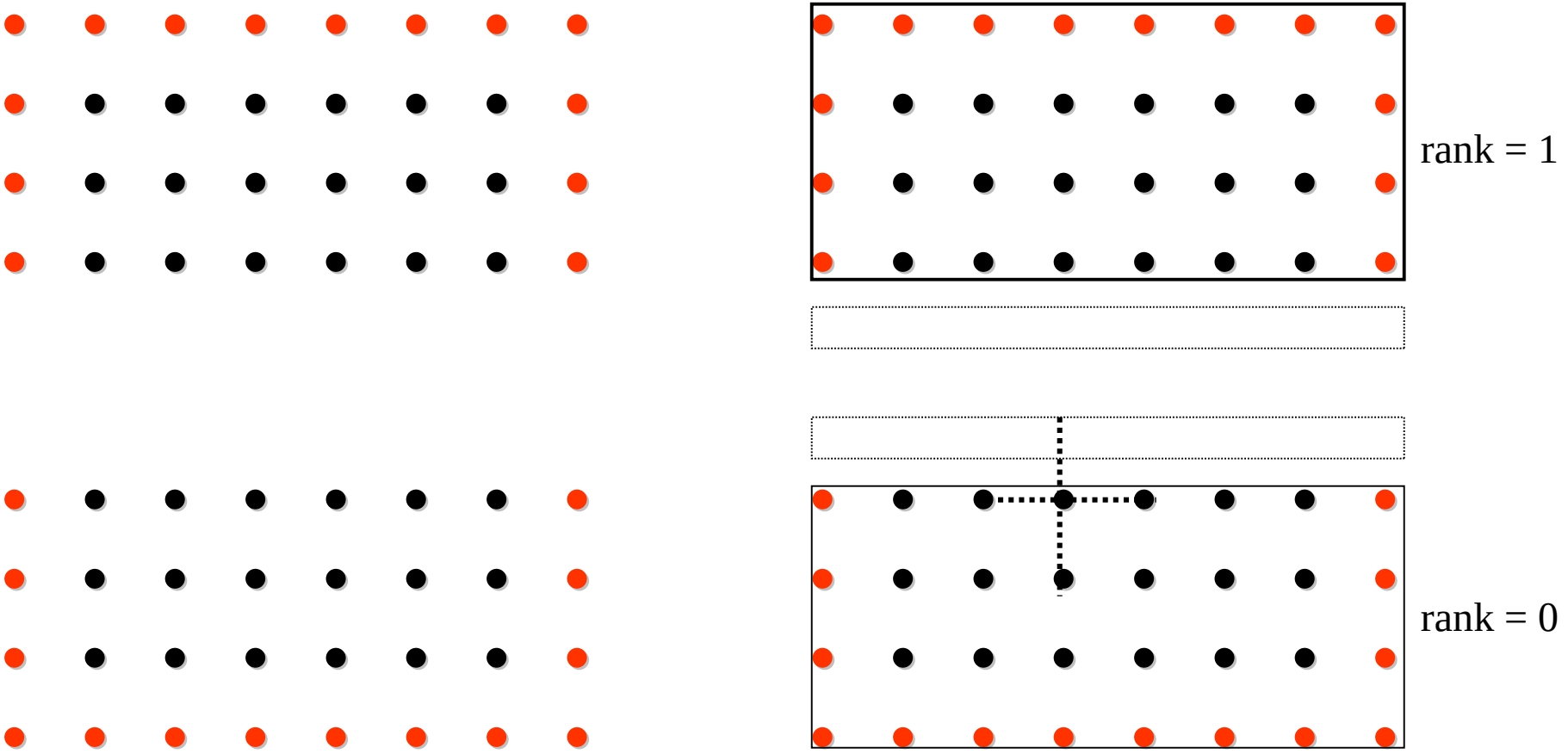
ψ(nx, ny)

ψ(nx, ny_local)

The “ghost” rows

i=2, nx-1 ; j=2, ny-1

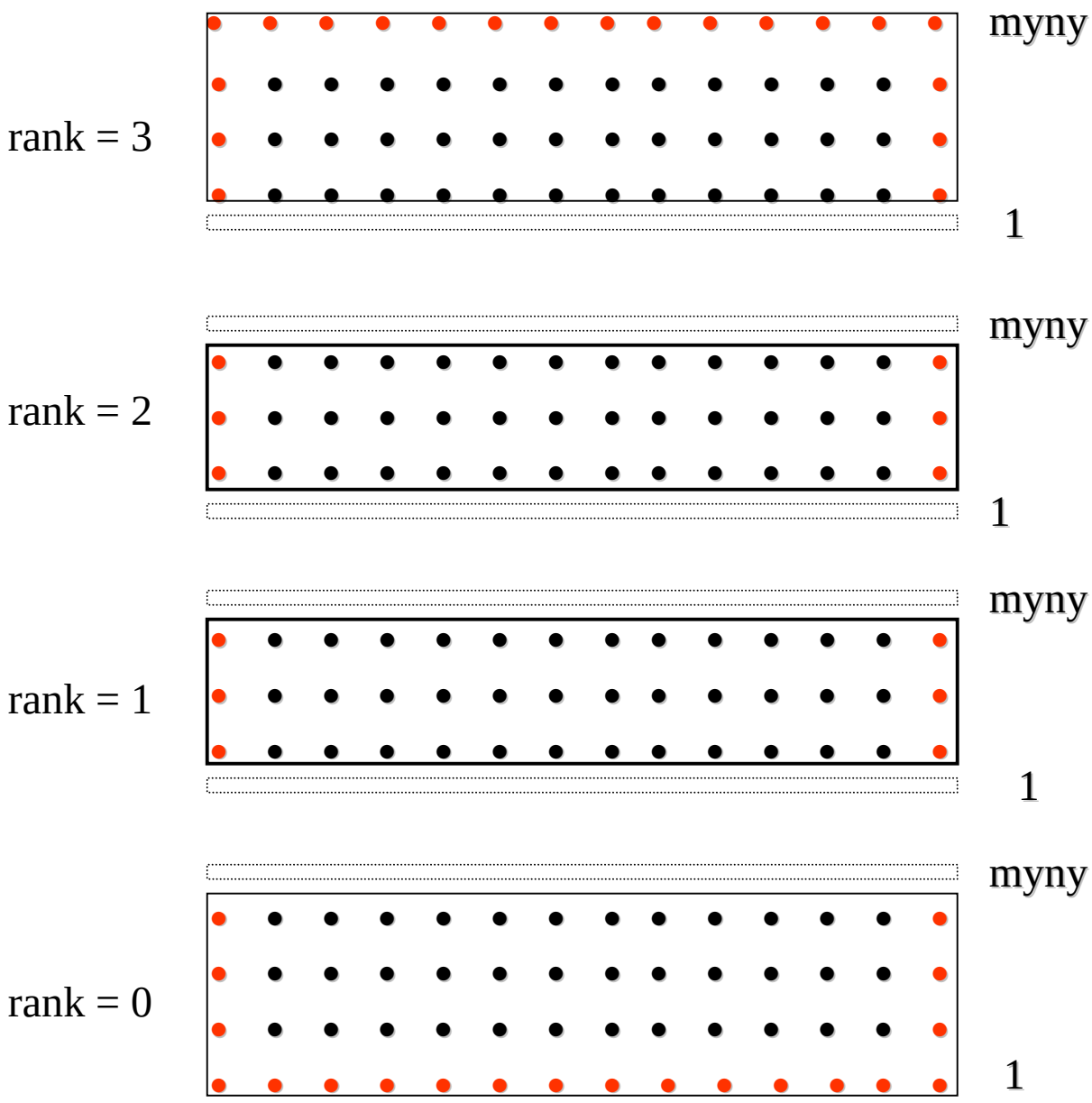
i=2,nx-1 ;j=2, myny-1



ψ(nx, ny)

ψ(nx, myny)

On defining "myny"



One choice:

myny = [(ny-2)/nprocs]

+ 2

STEP2: 1d decomposition of the arrays in the serial code

10 minutes

- cd /mpi1d_step2
- edit step2.f ….. (step2.f = step1.f + comments)

  - declare integer variable nprocs
  - for now set parameter(nprocs=1)
  - declare integer variable myny
  - set parameter(myny = [(ny-2)/nprocs] + 2])

STEP2: 1d decomposition of the arrays in the serial code (continued)

12 minutes

- edit /mpi1d_/step2/ step2.f ….. (continue)
  - change ny to myny everywhere in the code (EXCEPT in subroutine grid and in the parameter statement)
- compile and run step2.f with np = 1

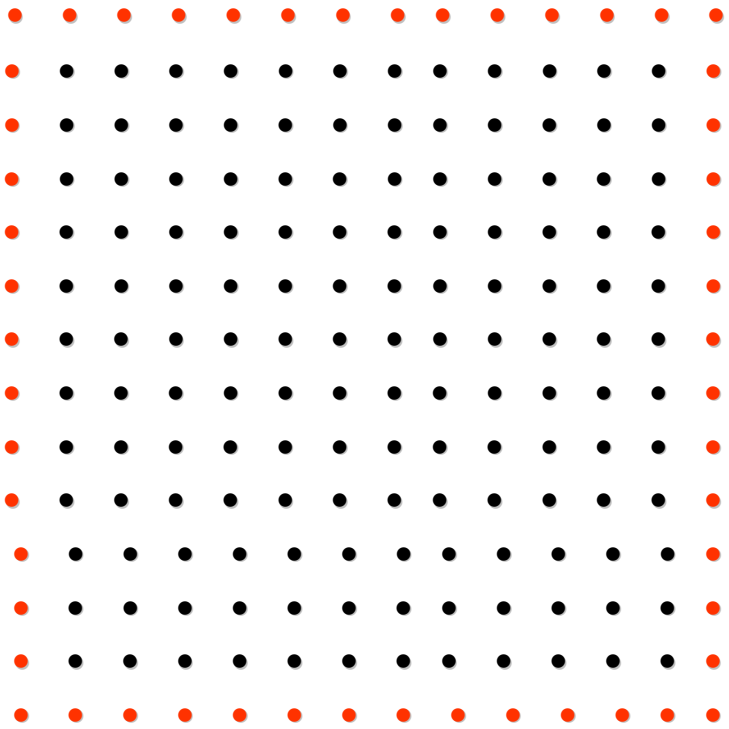
Decomposing the Forcing Function

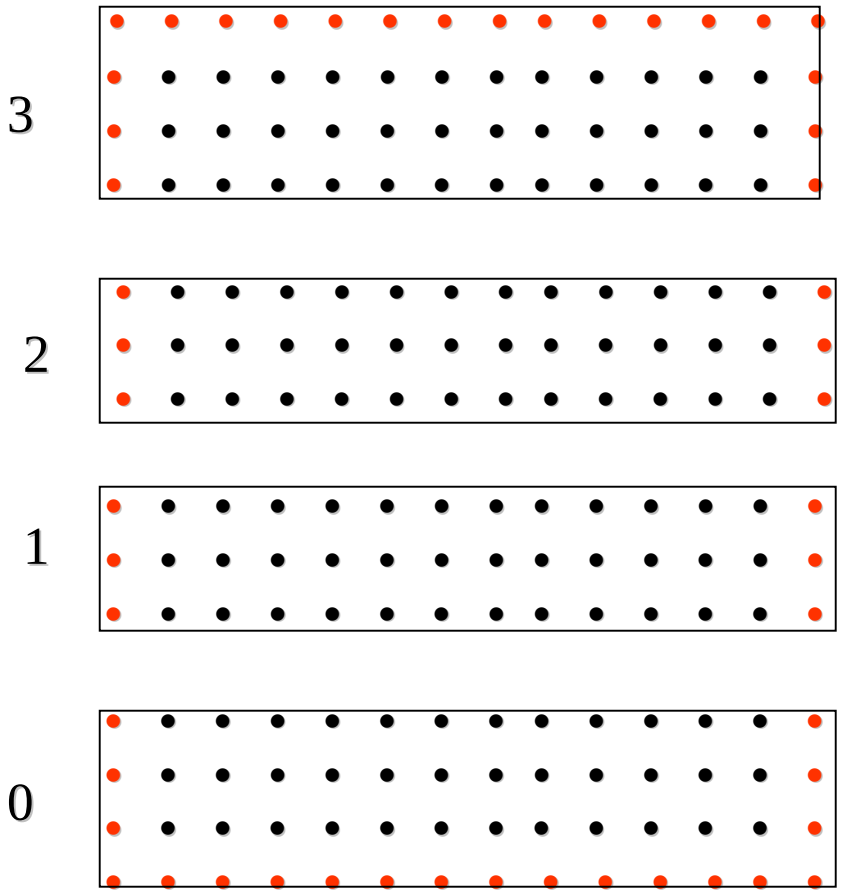
$$f(i,j) = -\alpha \sin(\pi * y(j)/Ly)$$

$yj = (j-1) * \Delta y$

$yj = ystart + (j-1) * \Delta y$

$ystart = rank * (myny-2) * \Delta y$





STEP3: decomposing the forcing function

8 minutes

- cd /mpi_1d/step3
- edit the file step3.f to make the following changes in routine “forcing”:

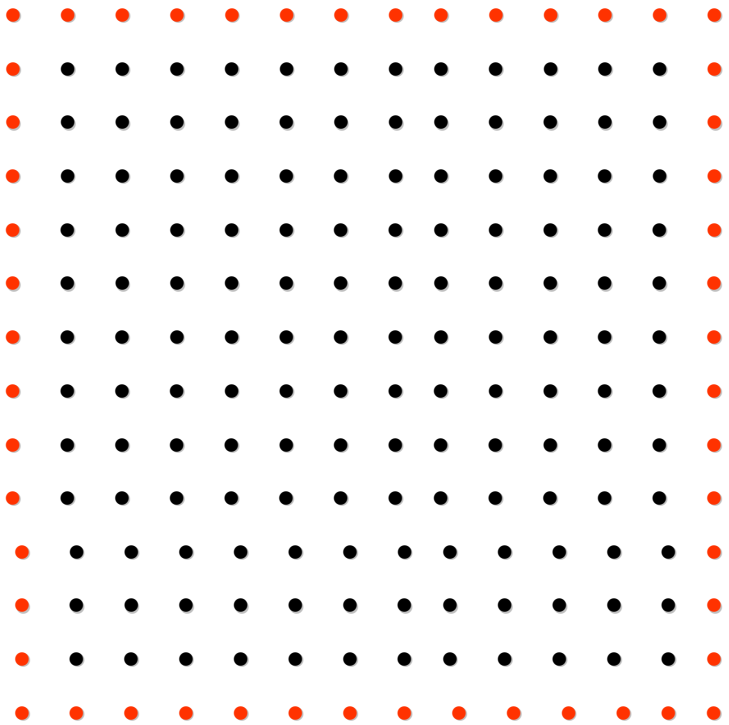
  - include rank as an argument of “forcing”
  - define ystart = rank * (myny-2) * dy
  - replace the statement for yj with

    yj = ystart + (j-1)* dy

- compile and run the code with np = 1

Decomposing the Horizontal Boundary Conditions

$\psi(i,ny) = 0 ; i = 1,nx$

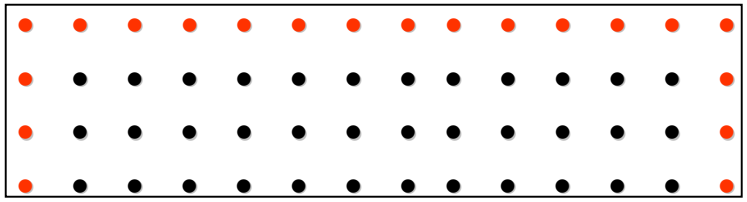


$\psi(i, 1) = 0 ; i = 1,nx$

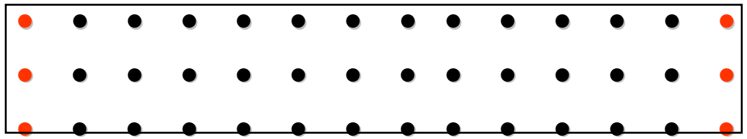
If (rank .eq. size-1)

$\psi(i,ny) = 0 ; i = 1,nx$

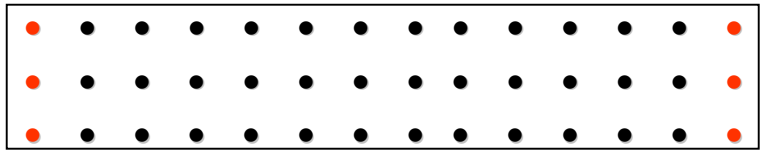
3



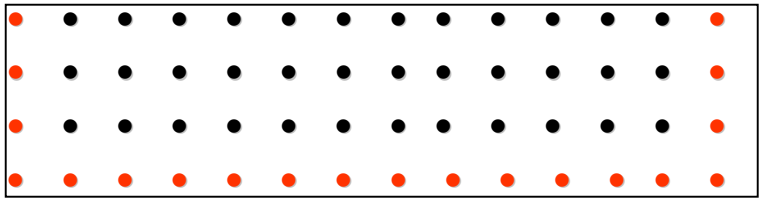
2



1



0



If (rank .eq. 0)

$\psi(i,1) = 0 ; i = 1,nx$

STEP4: Decomposing the Horizontal Boundary conditions

5 minutes

- cd /mpi1d_step4

- edit the file step4.f to make the following changes in the routine “bcs”:

  - include rank and size as arguments of “bcs”

STEP4: Decomposing the Horizontal Boundary conditions

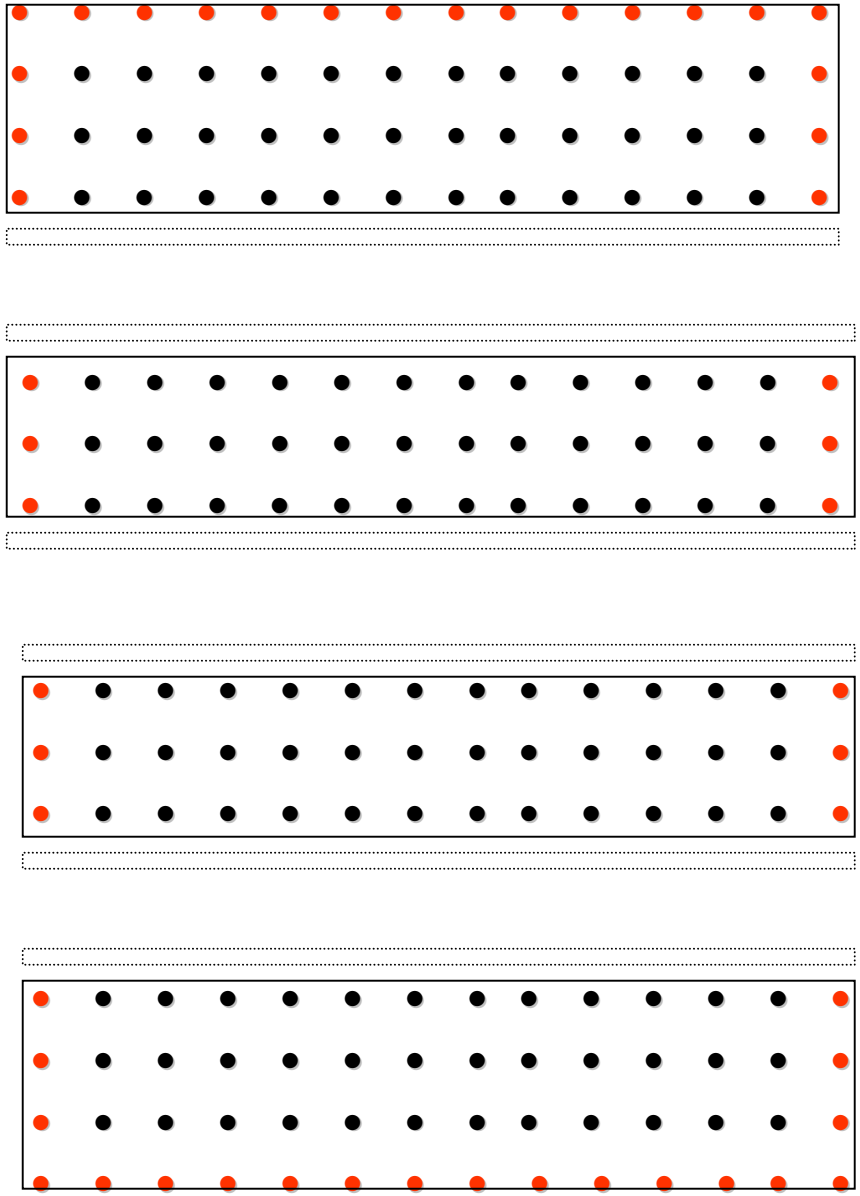
5 minutes

- split the do loop in bcs for x-boundaries into two loops: one for j = 0 and the other for j = myny

- set $\psi(i, 1) = 0$; i = 1, nx only if rank = 0
- set $\psi(i, myny) = 0$; i = 1, nx only if rank = size-1

- compile and run the code with np = 1

Who are my neighbors ?



rank of my neighbor above
=
my_rank+1

rank of my neighbor below
=
my_rank-1

STEP5: finding the ranks of neighbors

3 minutes

- cd /mpi-1d/step5

- edit the file neighbors.f :

  -modify the routine so that it will take rank as input and return integers "up" and "down" where up = rank + 1 & down = rank - 1

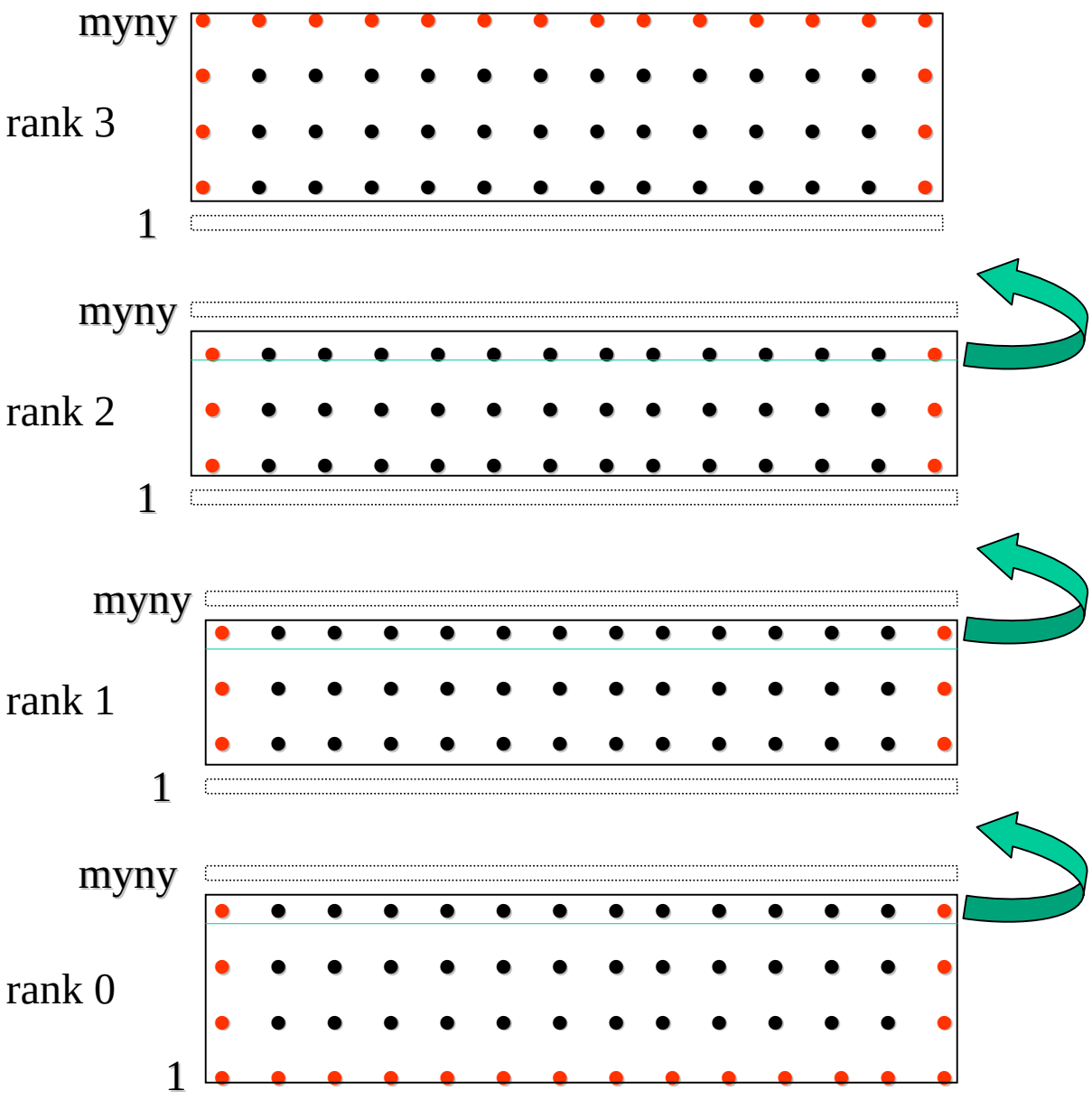
STEP6: Exchange the "Ghost Data" Across the Processors

3 minutes

cd /mpi_1d/step6

- edit the file exchange.f
  - include the mpi header file
  - declare two status arrays: status1 and status2 (integer type, with dimension MPI_STATUS_SIZE)

Exchanging the Ghost Data - (i)



If(rank .lt. size-1)send the last ”interior” row (i.e.ψ(i, myny-1)) to processor above

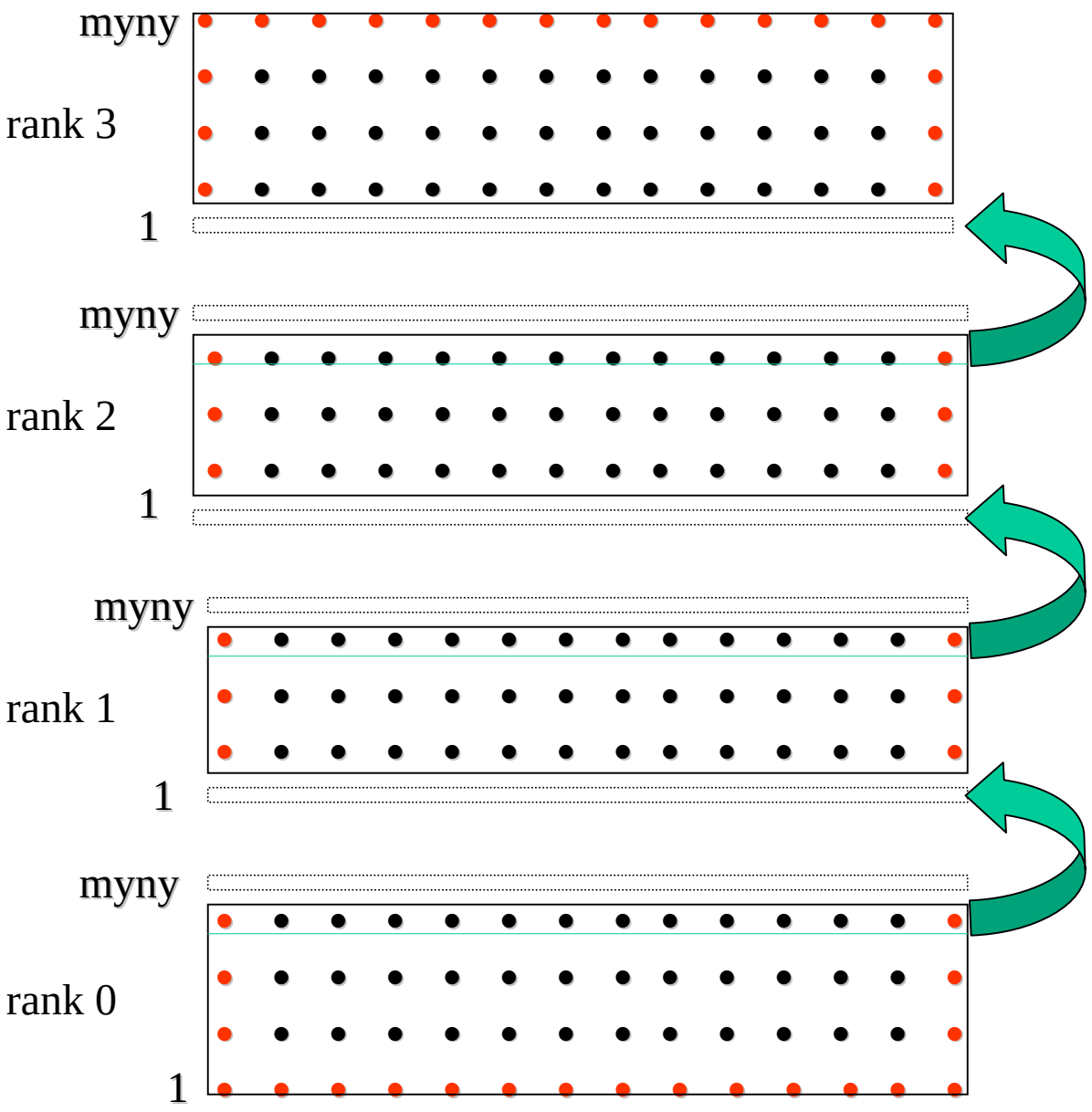
STEP6a: sending (myny-1)th row to the processor above

4 minutes

- cd mpi-1d/step6
- edit the file exchange.f to include the following MPI_SEND call at the indicated location.

```
CALL MPI_SEND(psi(1,myny-1),
                    nx,
                    MPI_REAL,
                    up,
                    999,
                    MPI_COMM_WORLD, ierr)
```

Exchanging the Ghost Data - (ii)



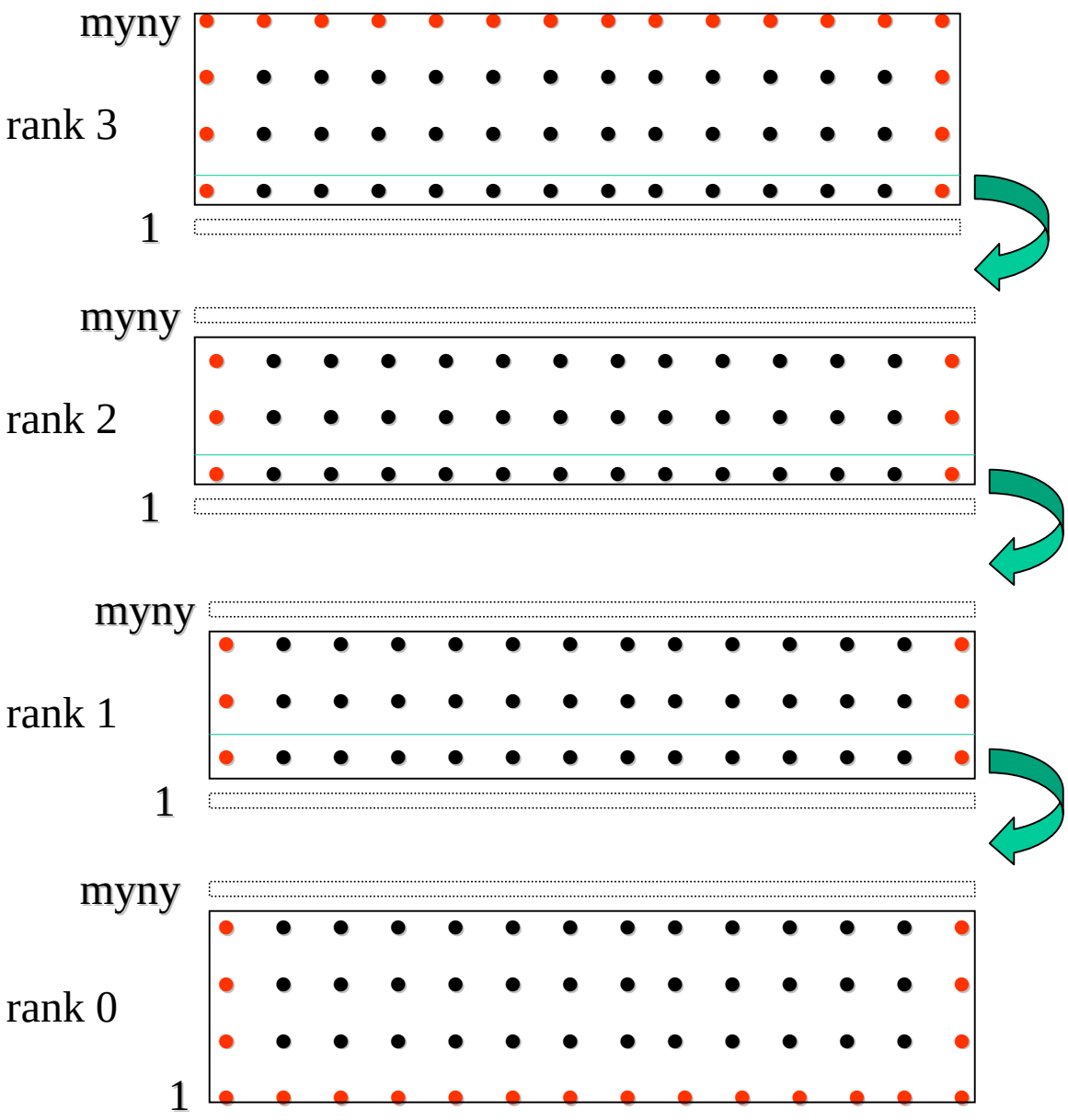
If(rank .gt. 0) receive a row of “real” type elements tagged 999 from the processor below and save it in the location starting at ψ(1,1)

STEP6b: receiving the first "ghost row" from processor below

4 minutes

- cd mpi-1d/step6
- edit the file exchange.f to include the following MPI_RECV call at the indicated location.
- CALL MPI_RECV(psi(1,1),
  nx,
  MPI_REAL,
  down,
  999,
  status1,
  MPI_COMM_WORLD, ierr)

Exchanging the Ghost Data - (iii)



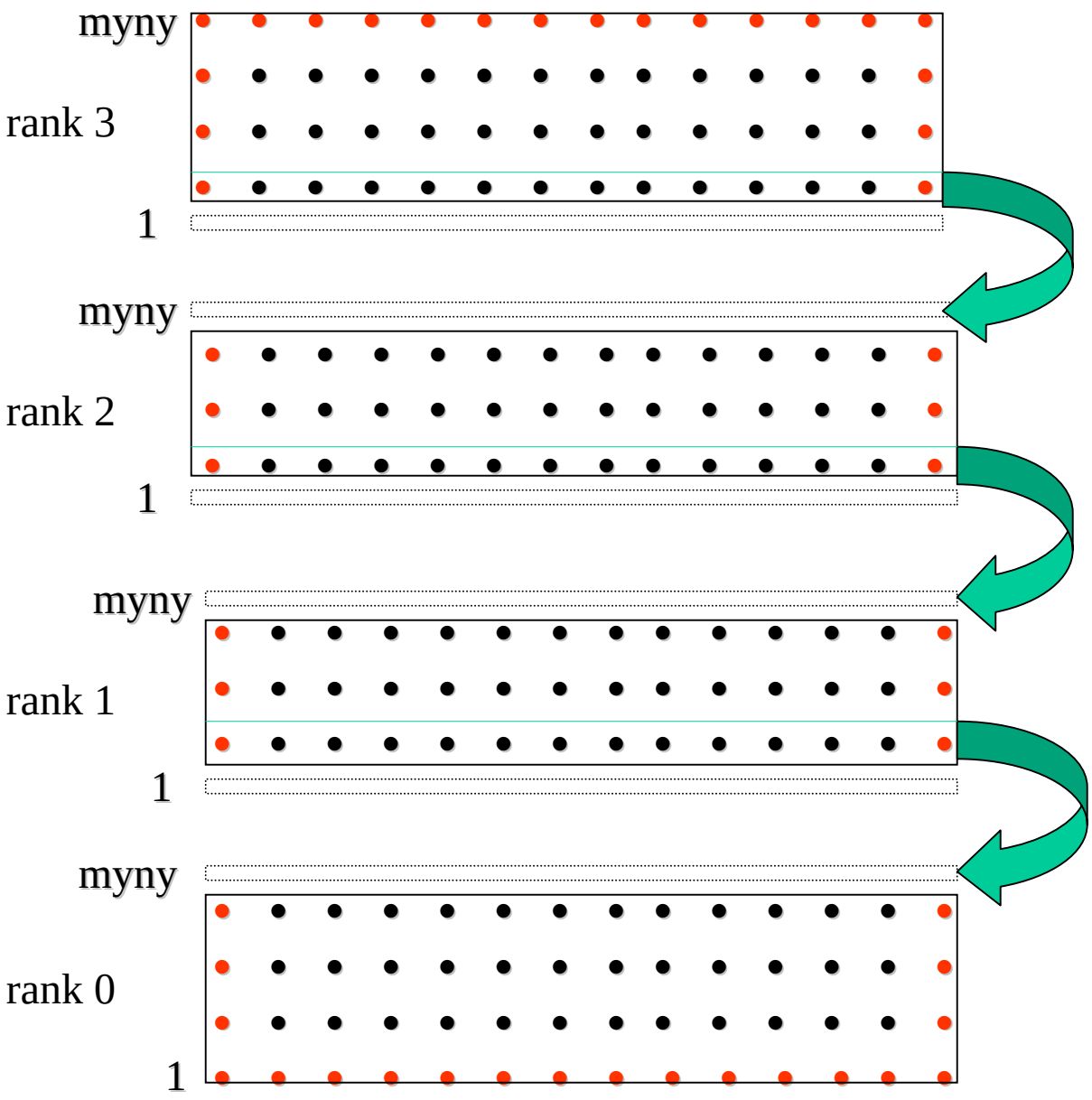
If(rank .gt. 0) send the first ”interior” row (i.e. ψ(i, 2)) to the processor below

STEP6c: sending the second row to the processor below

4 minutes

- cd mpi-1d/step6
- edit the file exchange.f to include the following MPI_SEND call at the indicated location.
- CALL MPI_SEND(psi(1,2),
  nx,
  MPI_REAL,
  down,
  888,
  MPI_COMM_WORLD, ierr)

Exchanging the Ghost Data - (iv)



If(rank .lt. Size-1) receive a row of "real" type elements tagged 888 from the processor above and save it in the location starting at ψ(1,myny)

STEP6d: receiving the last "ghost row" from processor above

4 minutes

- cd mpi-1d/step6

- edit the file exchange.f to include the following MPI_RECV call at the indicated location.

STEP6d: receiving the last "ghost row" from processor above (continued)

- CALL MPI_RECV(psi(1,myny),
  nx,
  MPI_REAL,
  down,
  888,
  status2,
  MPI_COMM_WORLD, ierr)

STEP6: a final check

1 minute

- cd /mpi-1d/step6
- compare your exchange.f with
  /mpi_1d/step6/completed/exchange.f

STEP7: Append neighbors.f and exchange.f to step4.f

4 minutes

- cd /mpi_1d/step7
- edit the file step7.f

  (step7.f = step4.f + neighbors.f + exchange.f +

  + additional comments)

  - declare integers up & below in the main program

  - insert a call to “neighbors” just before starting the iteration.

STEP7: Append neighbors.f and exchange.f to step4.f (continued)

4 minutes

- cd /mpi_1d/step7
- - insert a call to “exchange” inside the iteration loop - just before calling jacobi
- compile and run your code, but still with np = 1

STEP8: collecting the local residuals and reducing it to a global value

4 minutes

- cd /mpi_1d/step8

- edit the file step8.f to make the following changes in the routine “residual”

  - include the mpi header file
  - declare a new real variable lnorm: for local norm
  - replace gnorm with lnorm in the rest of the routine EXCEPT in the sqrt statement

STEP8: collecting the local residuals and reducing it to a global value (continued)

8 minutes

- use MPI_ALLREDUCE to collect the local residuals, to reduce it to a global value through a pre-defined operation and to distribute it back to all processors.

STEP8: collecting the local residuals and reducing it to a global value (continued)

- CALL MPI_ALLREDUCE(local buffer (lnorm),
  global value to be received (gnorm),
  # of elements in local buffer (1) ,
  datatype (MPI_REAL),
  reduction operation (MPI_SUM),
  MPI_COMM_WORLD, ierr)

- insert the call in residual - before computing sqrt
- compile and run the code, but still with np = 1

Step9 : The (Almost) Final Step

8 minutes

- cd /mpi_1d/step9

- edit step9.f to make the following changes in the main program
  - set nprocs = 4 (finally !!)
  - modify the print statement so that only processor 0 prints the output

- compile and run the code with np = 4

Residuals from the serial code and the mpi_1d version- What happened here ?

it_cnt	Serial Code	mpi_1d
1	1169699.38	1169729.5
2	1167068.75	1167098.12
3	1165272.38	1165305.12
4	1163841.5	1163839.38
5	1162584.12	1162584.12
6	1161434.	1161446.88
7	1160383.62	1160407.75
8	1159442.88	1159423.75
9	1158526.38	1158516.88
10	1157625.25	1157664.

Residuals from the serial code and the mpi_1d version- What happened here ?

Hint: sensitivity to the order of summation

STEP10:The Finishing Touch

4 minutes

- cd /mpi_1d/step10
- edit stml_serial.f to make the following changes in the routine residual:

-comment out gnorm=gnom+[ψ(i,j)-ψ_new(i,j)]**2

- insert gnorm=max (gnorm, abs(ψ(i,j)-ψ_new(i,j)))

- comment out gnorm = sqrt(gnorm)

- compile and run this modified version of stml_serial.f

STEP10: The Finishing Touch (continued)

- 4 minutes
- edit the file step10.f to make the following changes in the routine “residual
  - -comment out the statement for lnorm
  - - replace it with

    lnorm = max(lnorm, abs(ψ(i,j)-ψ_new(i,j)))
  - - comment out gnorm = sqrt(gnorm)

STEP10: A Finishing Touch (continued)

- 2 minutes

  - compile and run the code with np = 4

  - How does the results compare with that of the modified stml_serial.f

- You can now rename step10.f to stml_mpi1d.f